

Quantum critical point with competing propagating and diffusive spin excitations

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Feedback effects due to spin fluctuation induced precursors in the fermionic quasiparticle spectrum are taken into account in the description of a quantum critical point of itinerant spin systems. A correlation length dependent spin damping occurs, leading to a dynamical scaling with $z \approx 1$ which non-trivially competes with the conventional spin wave behavior. We obtain, within a one loop renormalization group approach, a quantitative explanation for the scaling behavior seen in underdoped cuprate superconductors.

Nuclear magnetic resonance (NMR) and inelastic neutron scattering (INS) experiments in magnetically underdoped cuprates [1–4] indicate that the spin excitations of these systems are close to a zero temperature quantum critical point (QCP) [5–9]. These measurements give strong indications for a dynamical scaling exponent $z \approx 1$, typical for systems characterized by propagating antiferromagnetic (AF) spin modes, but different from that expected for an itinerant AF system with $z = 2$ [5,7,9]. On the other hand, the low frequency behavior of the imaginary part of the dynamical spin susceptibility is characterized by over-damped spin-excitations, i.e. $\text{Im}\chi(\mathbf{q}, \omega) \propto \omega + \mathcal{O}(\omega^3)$, as expected for itinerant AF. Thus, while the spin dynamics is clearly over-damped, the scaling behavior corresponds to that of a system without damping, causing a conceptual problem for the description of the related QCP.

In the present paper we investigate the behavior in the vicinity of a QCP characterized by competing propagating and diffusive spin excitations. We explicitly take into account that for a system characterized by strong interactions between collective spin modes and fermionic quasiparticles the latter are strongly affected by the critical mode. This, in turn, leads to a feedback in the spin dynamics [10,11], causing $z \approx 1$ dynamical scaling behavior for an itinerant AF. Our theory offers a quantitative explanation for the temperature and frequency dependence of INS and NMR data and confirms the phenomenological description of the spin dynamics of Refs. [1,2].

We start from an interacting Fermi system characterized by some unperturbed band-part and an interaction term, $\sum_{\mathbf{q}} f_{\mathbf{q}} \mathbf{s}_{\mathbf{q}} \cdot \mathbf{s}_{-\mathbf{q}}$, with fermionic spins, $\mathbf{s}_{\mathbf{q}} = \frac{1}{2} \sum_{\mathbf{k}\sigma\sigma'} c_{\mathbf{k}+\mathbf{q}\sigma}^\dagger \sigma_{\sigma\sigma'} c_{\mathbf{k}\sigma'}$. By introducing a collective spin-1 Bose field, $\mathbf{S}(\mathbf{q})$, via the Hubbard-Stratonovich transformation, one can integrate out the fermions and expand up to forth order in $\mathbf{S}(\mathbf{q})$ [12]; the resulting effective action of the collective spin degrees of freedom is [5,7]:

$$S = \frac{1}{2} \int^\Lambda d\mathbf{q} \chi_0^{-1}(\mathbf{q}) \mathbf{S}(\mathbf{q}) \cdot \mathbf{S}(-\mathbf{q})$$

$$+u \int^\Lambda d\mathbf{q}_1 \cdots \int^\Lambda d\mathbf{q}_4 \delta_{\mathbf{q}_1+\mathbf{q}_2+\mathbf{q}_3+\mathbf{q}_4} \times \mathbf{S}(\mathbf{q}_1) \cdot \mathbf{S}(\mathbf{q}_2) \mathbf{S}(\mathbf{q}_3) \cdot \mathbf{S}(\mathbf{q}_4), \quad (1)$$

characterized by a bare spin propagator, $\chi_0(\mathbf{q})$, and coupling constant, $u > 0$. In Eq. 1 the $(d+1)$ -dimensional vector $\mathbf{q} = (\mathbf{q}, i\omega_n)$ consists of the d -dimensional momentum vector \mathbf{q} and the bosonic Matsubara frequency $\omega_n = 2n\pi T$ at temperature, T . We write $\int^\Lambda d\mathbf{q} \cdots = T \sum_n \int_{|\mathbf{q}| < \Lambda} \frac{d^d \mathbf{q}}{(2\pi)^d} \cdots$ and $\delta_{\mathbf{q}+\mathbf{q}'} = T^{-1} \delta_{n+n'} \delta^{(d)}(\mathbf{q} + \mathbf{q}')$, where Λ is the upper momentum cut off. A diagrammatic representation of this action is given in Fig. 1(a).

Usually, $\chi_0(\mathbf{q})$ and u are calculated within a weak coupling approach in which the spin damping due to particle hole excitations is identical to that of a noninteracting electron gas [5,7] (see Fig. 1(b)). It is however to be expected that the fermionic quasiparticles are strongly affected by their own spin excitations once the system gets close to a magnetic instability [11,13–15]. It is therefore interesting to take into account these modifications of the quasiparticle spectrum in an investigation of the critical behavior. Of particular importance are quasiparticles close to the magnetic BZ-boundary, which, on the one hand, determine the spin damping, $\gamma \propto \text{Im}\chi^{-1}(\mathbf{Q}, \omega)/\omega|_{\omega \rightarrow 0}$, and, on the other hand, are mostly affected by the proximity to the ordered state.

Magnetic precursors in the quasiparticle spectrum have recently been investigated in several theories [11,13–15]. Within a quasistatic theory [11], applicable at higher T , γ was calculated to all orders in the perturbation theory. Due to precursors of a spin density wave (SDW) gap the low energy spectral weight is reduced and the vertex function enhanced and γ was found to change from being a constant to a ξ -dependent function: $\gamma \propto \xi^{-\varphi}$ with $\varphi \approx 1$, once ξ is larger than the electronic length scale, $\xi_0 = 2v/f_{\mathbf{Q}}$. In cuprates $\xi_0 \approx 2$ due to the large coupling constant $f_{\mathbf{Q}}$. For low temperatures the situation is more complicated [16,17]. Nevertheless, the leading contribution to the spin damping can be estimated as $\gamma \propto f_{\mathbf{Q}}^2 \Gamma^{\text{sf}}/v^2$, with spin fermion vertex function at the Fermi surface (FS) and for momentum trans-

fer $\mathbf{Q} \approx (\pi, \pi)$, Γ_{sf} , and Fermi velocity, v . At the critical point the vertex function for scattering processes including a Goldstone mode is expected to vanish on a surface defined by momentum and energy conservation of the involved quasiparticles [18]. In the case of large correlation length and large interaction $f_{\mathbf{Q}}$, a FS evolution towards an SDW like behavior occurs and the above principle causes the vertex function to vanish like $\Gamma_{\text{sf}} \propto \xi^{-1}$ [14], leading to $\gamma \propto \xi^{-1}$. Thus, we expect in various regimes a ξ -dependent reduction of the spin damping due to the proximity to an ordered state.

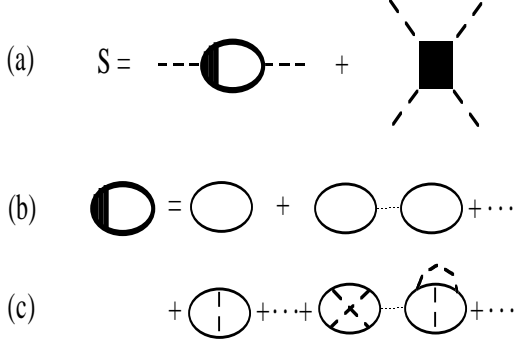


FIG. 1. (a) Diagrammatic representation of the effective action with spin-propagator and spin spin interaction term. The dashed lines correspond to collective spin degrees, the solid lines to the renormalized fermionic Green's function. (b) Typical weak coupling approximation for $\chi_0(q)$. Dotted lines refer to the fermion-fermion interaction, $f_{\mathbf{q}}$. (c) Some of the diagrams causing feedback effects of the quasiparticle excitations.

In the present communication we take these feedback effects into account and determine $\xi(T)$ using a renormalization group approach. The propagator of the collective spin modes is assumed to be:

$$\chi_0(\mathbf{q}, i\omega_n) = \frac{\alpha}{\xi_0^{-2} + \mathbf{q}^2 + \xi_0^{-\varphi} |\omega_n| / \hat{c} + (\omega_n/c)^2}, \quad (2)$$

with bare correlation length ξ_0 , spin damping, $\gamma = \hat{c}^{-1} \xi_0^{-\varphi}$ and spin wave velocity c . Momenta are measured relative to the ordering vector. For $\hat{c} \rightarrow \infty$, i.e. without spin damping, the problem is similar to that investigated by Chakravarty *et al.* [6] and Chubukov *et al.* [8]. The alternative limit $\varphi = 0$ and $c \rightarrow \infty$ was discussed by Hertz [5] and Millis [7]. The case $\varphi = 0$ but c finite was discussed by Sachdev *et al.* [9], who found a $z = 1$ to $z = 2$ crossover for decreasing temperature, in contrast to the experimental finding in the cuprates of a $z = 2$ to $z = 1$ crossover for decreasing T [1,2,4].

We use a Kadanoff-Wilson momentum shell renormalization group approach; integrating out states with momenta between Λe^{-l} and Λ , including the rescaling $T(l) = e^{zl} T$ to reach self-similarity. Up to one loop the resulting flow equations are:

$$\frac{dT(l)}{dl} = zT(l) \quad (3)$$

$$\frac{d\xi_0^{-2}(l)}{dl} = 2\xi_0^{-2}(l) + 4(N+2)u\Phi(\xi, T(l)) \quad (4)$$

$$\frac{du(l)}{dl} = \epsilon u(l) - 4(N+8)u^2\Psi(\xi, T(l)) \quad (5)$$

$$\frac{d\hat{c}(l)}{dl} = (z + \varphi - 2)\hat{c}(l) \quad (6)$$

$$\frac{dc(l)}{dl} = (z - 1)c(l), \quad (7)$$

with $\epsilon = 4 - (d + z)$. N is the number of vector components of $\mathbf{S}(q)$. The functions Φ and Ψ can be determined along the same lines as in Ref. [7]. Their explicit dependence on the renormalized correlation length, ξ , results from a replacement of ξ_0 by ξ in diagrams like those in Fig. 1(c) which determine the spin damping, necessary to reach self consistency [19]. From Eqn. 6 and 7 we find that for $\varphi = 1$ (i.e. $z = 1$) the velocities \hat{c} and c do not renormalize in the one loop approximation. In the case $\varphi < 1$ one starts from a primary scaling behavior with $z = 1$ which eventually crosses over to $z = 2 - \varphi$ [9]. In what follows we assume $\varphi = 1$ since quantitatively the latter crossover will barely change our results; an extension to arbitrary φ is straightforward. Moreover, small deviations from $z = 1$ seem to be beyond the accuracy of the current experiments. For $\epsilon > 0$ the flow equations, Eqn. 3 - 7, are characterized by a zero temperature fixed point $(\xi_0^*)^{-2} = -\frac{N-2}{N-8}\epsilon\Lambda^2$ and $u^* = \Gamma(d/2)2^{d-1}\pi^{d/2}\epsilon/((N+8)c\Lambda^{d-3})$, which is unstable since T is a relevant field. By integrating the flow equations we find that the critical behavior is sufficiently characterized by the single effective coupling constant $g = 2(1-d)(N+2)u\xi_0^2$. This is also expected since the critical behavior should be similar to that of the quantum nonlinear sigma model which is fully characterized by g and T [6,8]. For $d = 2$, the fixed point value of g is given by $g^* = 4\pi/(c\Lambda)$, which is unchanged from the result without damping [6,8] (the limit $\hat{c} \rightarrow \infty$). Nevertheless, the critical behavior in the vicinity of this QCP depends strongly on the ratio, $\Gamma \equiv c/\hat{c}$. In the limit $c \rightarrow \infty$ the QCP moves towards $g^* = 8\pi/\Lambda_\omega$ with upper frequency cut off Λ_ω . The flow equations, Eqn. 3 - 7, can be integrated and the correlation length follows from $\xi = e^l \xi(g(l), T(l))$, where we determine the correlation length at the matching point [6], $l = \bar{l}$, with $T(\bar{l}) = c\Lambda/4$ and $g(\bar{l}) = 2g^*$ from a $1/N$ expansion as used in Ref. [8]. Note, since $g(l)$ depends on ξ , this procedure leads to a self consistency condition for ξ .

The QCP, g^* , separates in the usual sense [6] a renormalized classical (RC) regime with exponentially growing correlation length, $\xi(T) = \hat{c}/(2T) \exp(2\pi c\Lambda/T(\frac{1}{g^*} - \frac{1}{g}))$, for $g(l=0) < g^*$, from a quantum disordered (QD) state with a finite zero temperature correlation length, $\xi(0)$, (see Fig. 2). We find for $\Gamma \gg 1$ that $\xi(0)/\log(\xi(0)\Lambda) = \frac{\Gamma g^*}{4\pi\Lambda}(g - g^*)^{-1}$, which is enhanced compared to the situation without damping: $\xi(0) = \frac{g^*}{2\Lambda}(g - g^*)^{-\nu}$ with $\nu = 1$

up to one loop. The results of a numerical evaluation of $\xi(0)^{-1}$ are shown in the inset of Fig. 2.

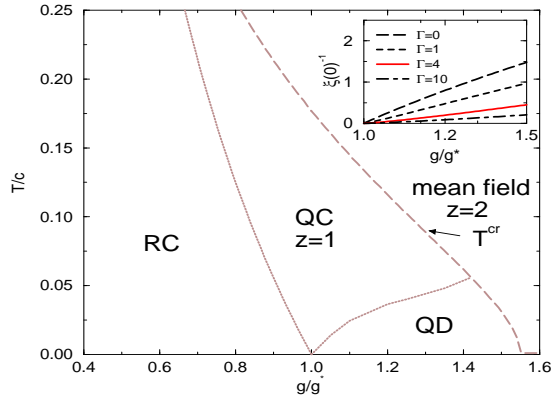


FIG. 2. Phase diagram of an itinerant AF with $z = 1$ scaling behavior for $\Gamma = 4$. RC is the renormalized classical regime with exponentially large ξ . QC is the quantum critical regime and QD the quantum disordered regime. In the mean field regime, $T > T^{cr}$, with $\xi < \xi_o \approx 2$ no feedback effect due to changed quasiparticle behavior occurs, leading to $z = 2$. The inset shows the inverse zero temperature correlation length in the QD regime for different Γ .

Modified scaling behavior can in similar fashion be found as function of temperature. In Fig. 3 we show our results for the T -dependent correlation length for $g/g^* = 1.18$ and different values of Γ . We find up to logarithmic corrections, $\xi(T)^{-2} \approx \xi(0)^{-2} + bT^2$ (see inset of Fig. 3(b)). In contrast, in the case of propagating spin excitations a sharp transition to an exponentially weak temperature dependent ξ occurs for $T \approx \Delta$ with spin wave gap $\Delta = c\xi(0)^{-1}$. Thus, due to spin damping the spin wave gap is filled with low energy states and the correlation length continues to grow even for very low temperatures. The crossover between the quantum critical (QC) and QD regime is very gradual. In Fig. 2 the crossover line was determined by the temperature where $d^2\xi^{-1}/dT^2$ becomes small compared to its low T value, i.e. where ξ^{-1} starts to grow linearly with T . Finally, considering higher temperatures, we have to take into account that $\gamma \propto \xi^{-1}$ occurs only for $\xi \geq \xi_o \approx 2$ [11]. For $\xi < \xi_o$, $\gamma = \text{const.}$ leading to a $z = 2$ behavior at a characteristic temperature T^{cr} (see Fig. 2).

Another characteristic phenomenon caused by the proximity to a QCP is the scaling behavior of the frequency dependence of $\text{Im}\chi(\mathbf{q}, \omega)$. For any point in the (T, g) phase diagram (except $g \leq g^*$ and $T = 0$) $\text{Im}\chi_{\mathbf{q}}(\omega)$ increases linearly with ω due to excitations in the particle hole continuum. In the RC regime however, the spin damping is exponentially suppressed and the spin dynamics is indistinguishable from a system with purely propagating spin waves. On the other hand, in the QC regime ω/T scaling behavior of $\xi^{-2}\text{Im}\chi_{\mathbf{q}=0}(\omega)$ and of

the momentum averaged susceptibility $\int d^2\mathbf{q} \text{Im}\chi_{\mathbf{q}}(\omega)$ is found and the low frequency slope of $\chi_{\mathbf{q}=0}(\omega)$ behaves like $\text{Im}\chi_{\mathbf{q}=0}(\omega)/\omega|_{\omega \rightarrow 0} = \alpha\xi^\delta/\hat{c}$ with $\delta = 3$.

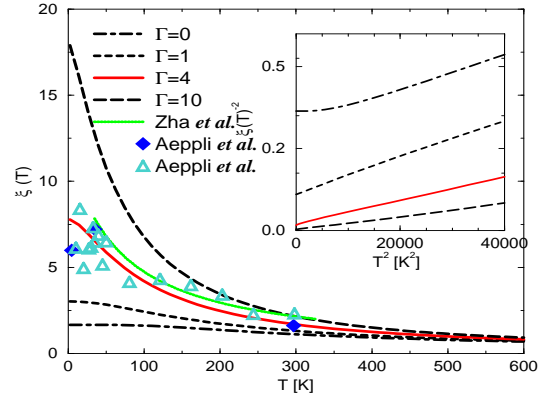


FIG. 3. Temperature dependence of the correlation length for $g = 1.18g^*$ and different Γ in comparison with experimental data for $\text{La}_{1.86}\text{Sr}_{0.14}\text{CuO}_4$ from Ref.[3] at $\omega = 2.5$ (3.5) meV indicated by diamonds (triangles) and the phenomenological theory of Ref.[2]. The inset shows $\xi(T)^{-2}$ versus T^2 .

In applying these results to cuprate superconductors, we assume that doped systems without long range order are located in the QC and QD regime. Since $g \propto 1/\langle \mathbf{S}(\mathbf{r})^2 \rangle$, as follows from a $1/N$ expansion, doping reduces the effective moment, causing the coupling constant to grow until it exceeds g^* . For the cuprate material $\text{La}_{1.86}\text{Sr}_{0.14}\text{CuO}_4$ the parameters $\hat{c} \approx 50$ meV and $c \approx 220$ meV are reasonably well known from NMR and INS experiments [1–3] and it follows $\Gamma \approx 4$. Thus, it suffices for a quantitative understanding of the INS data of Ref [3] to determine the ratio g/g^* from the correlation length at a given temperature. Once this number is determined one has a complete description of the T - and ω -dependence of the spin fluctuation spectrum. As shown in Fig. 3, a value $g = 1.18g^*$ gives a reasonable agreement not only for the value of ξ at low T but also for the whole temperature regime up to 300 K. Using this value for the coupling constant we can determine the frequency and temperature dependence of the dynamical spin susceptibility. The results for $\text{Im}\chi_{\mathbf{q}=0}(\omega)$ with $\alpha = 26 \text{ eV}^{-1}$, shown in Fig. 4, are in remarkable agreement with the results of Aeppli *et al.* [3], who also find $\text{Im}\chi_{\mathbf{q}=0}(\omega)/\omega|_{\omega \rightarrow 0} \propto \xi^\delta$ with $\delta = 3 \pm 0.3$. This agreement between theory and experiment is a direct consequence of the fact that the experimental data show a ω/T scaling behavior of $\xi^{-2}\text{Im}\chi_{\mathbf{q}=0}(\omega)$ which is a strong indication that the system under consideration is indeed close to a QCP. In order to demonstrate that our results agree quantitatively with the phenomenological description of the $z = 1$ pseudo-scaling regime of Ref. [2], we also show in Fig. 3 the correlation length, $\xi(T)$, as obtained from

NMR experiments [20].

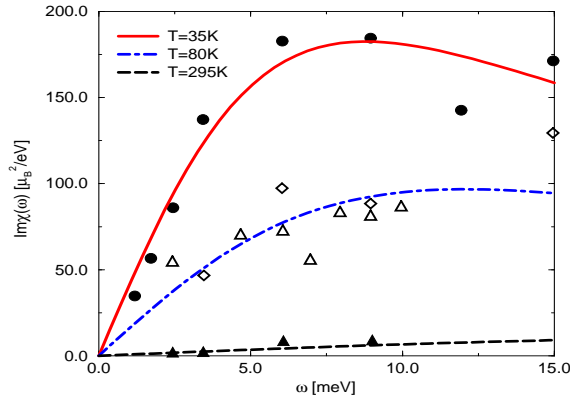


FIG. 4. Frequency dependence of the dynamical susceptibility at the peak maximum for $\Gamma = 4$ and $g = 1.18g^*$ in comparison with INS experiments from Ref.[3].

In conclusion, based on previous calculations [11,13–15], we have argued that modifications of the particle hole excitation spectrum can change the dynamical scaling behavior of itinerant AF systems close to a QCP by affecting the spin damping. The resulting $z \approx 1$ scaling causes a T -dependence of the AF correlation length which is completely different from the usual $z = 2$ case. This new T -dependence of the dynamical spin susceptibility is in remarkable agreement with NMR and INS experiments and gives an explanation for the crossover scenario of Refs. [1,2]. The $z = 1$ scaling and the position of the QCP are the same as those for propagating spin modes in insulating AF. However, due to damping, the correlation length is enhanced and the T -dependence of ξ is changed.

We expect similar behavior in the quantum phase transitions of other itinerant systems if the strong interaction between quasiparticles and collective modes changes the dynamics of the collective mode under consideration. Examples are one and two dimensional charge density wave systems, superconductors or saturated ferromagnets. In higher dimensions or for systems with weak quasiparticle-collective mode coupling precursor phenomena are only expected once ξ diverges [15] and will play no role in the quantum disordered regime.

Finally, we note that the theory presented in this paper is not a theory for the crossover to a *strong pseudogap* state found in many cuprate superconductors at low T , where a decoupling of the T -dependence of ξ and γ has been found [1,4]. This might be due to the interference with excitations different from the spin fluctuation channel discussed here [17,21]. Nevertheless, we expect the proximity to a QCP to be essential for the appearance of the strong pseudogap behavior.

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